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Strategies to design materials for electrochemical energy conversion and storage technologies

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Abstract

The development of novel materials for electrodes and catalysts is still an important research activity for solid state or high temperature electrochemical cells, such as solid oxide fuel cells and electrolyzers. Also in case of batteries the search for new/ advanced or improved materials is still ongoing. The presentation will strive some strategies for materials development, based on considerations of the electrochemical processes occurring in electrode materials and especially at the electrode/ electrolyte interface. There examples will be addressed:

Fuel electrodes for solid oxide fuel cells: In to overcome the limitation of the fuel oxidation at only triple phase boundaries in state-of-the-art Ni-cermet electrodes, ceramic electrodes based on mixed electronic and ionically conducting materials have been suggested to increase the electrochemically active area in the electrode. This development has led more recently to the design of ceramic electrodes with nanostructured electro catalysts, which also may offer more tolerance to coking and sulphur poisoning.

Air electrodes in solid oxide cells: The oxygen exchange reaction at perovskite ceramics is a central mechanism in these electrodes. While often for perovskites the surface exchange is related to the oxygen diffusion in the bulk material, recent results point also to the importance of the electronic properties of the materials. A structural field map approach for perovskites has been proposed based on the observation that the most interesting air electrode materials seem to be border region between metallic and semiconductors, which is influenced by the perovskite A and B cation size.

High voltage cathode materials for Li-batteries: Increasing the energy density in batteries is a crucial point for their future application esp. as regards automotive applications. The NaSiCon structure is very robust and a li-Fe Phosphate has been proposed to be able to sustain the transition from Fe2+ to Fe3+ to Fe 4+. However, despite of stable charging and discharging behavior, the desired high voltage operation was not achieved. In combination of operando XRD and DFT modelling the reason for this limitation has been analyzed, which gives new hints to further modify the material to achieve the desired high voltage operation.

Besides operando characterization and modelling, electrochemical impedance spectroscopy has been a powerful tool in all three approaches to support the development and evaluate the resulting materials. The presentation aims at stimulating a discussion on design strategies and the role of EIS but also perspectives and limitations of complementary characterization and modelling techniques for a more rational approach to novel or improved materials.